

# PUBCHEM\_54605649

40730-78-7 | DTXSID90714109

## Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

## Model Results

**Predicted value:** 1.65e-01 mol/L

**Global applicability domain:** Inside

**Local applicability domain index:** 3.61e-01

**Confidence level:** 6.35e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Taurocyamine

**Measured:** 2.33e-01

**Predicted:** 3.13e-01

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2-amino-3-(4-chlorophenyl)sulfonylpropanoic acid

**Measured:** 2.93e-03

**Predicted:** 7.20e-02

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1H-Imidazole-5-sulfonic acid

**Measured:** 1.35

**Predicted:** 7.40e-01

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1H-Imidazole-2-sulfonic acid

**Measured:** 8.44e-01

**Predicted:** 7.41e-01

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Benzenesulfonic acid, 3-hydrazino-

**Measured:** 1.49e-01

**Predicted:** 5.98e-01